

Coupled-cluster approaches to nuclear quantum many-body problems

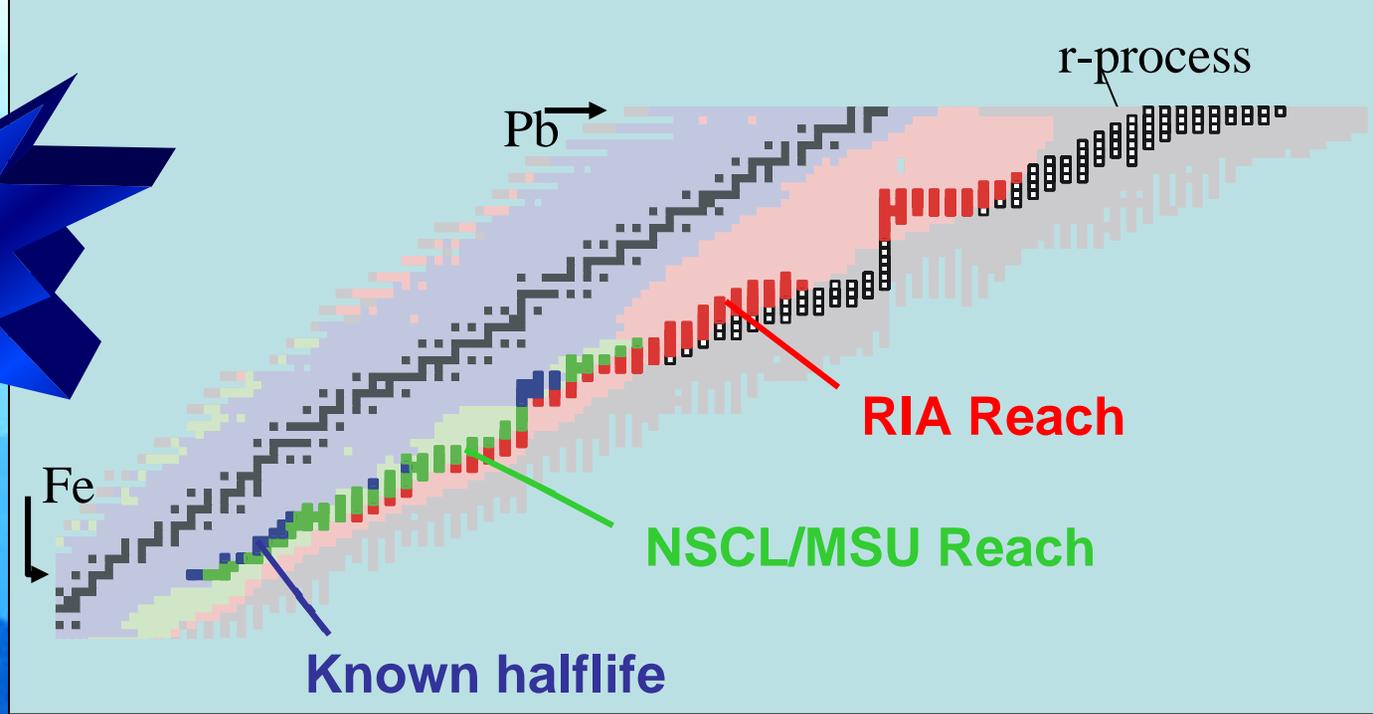
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ORNL

Outline

- I. Perspective
- II. Coupled-cluster theory – a path forward
 - A. The space and the Hamiltonian
 - B. The CC method in single and double excitations (CCSD)
 - C. Triples corrections and excited states
 - D. Open issues
- III. Future directions

RIA is coming

Feb 04: CD-0
Site selection



Scientific Thrusts:

- How do complex systems emerge from simple ingredients (interaction question)?
- What are the simplicities and regularities in complex systems (shell/symmetries question)?
- How are elements produced in the Universe (astrophysics question)?

Broad impact of neutron-rich nuclei:

- Nuclei as laboratories for tests of ‘standard model physics’.
- Nuclear reactions relevant to astrophysics.
- Nuclear reactions relevant to Science Based Stockpile Stewardship.
- Nuclear transportation, safety, and criticality issues.

Theory research opportunities:

2004 NSAC report “A vision for nuclear theory”

Structure/reaction developments

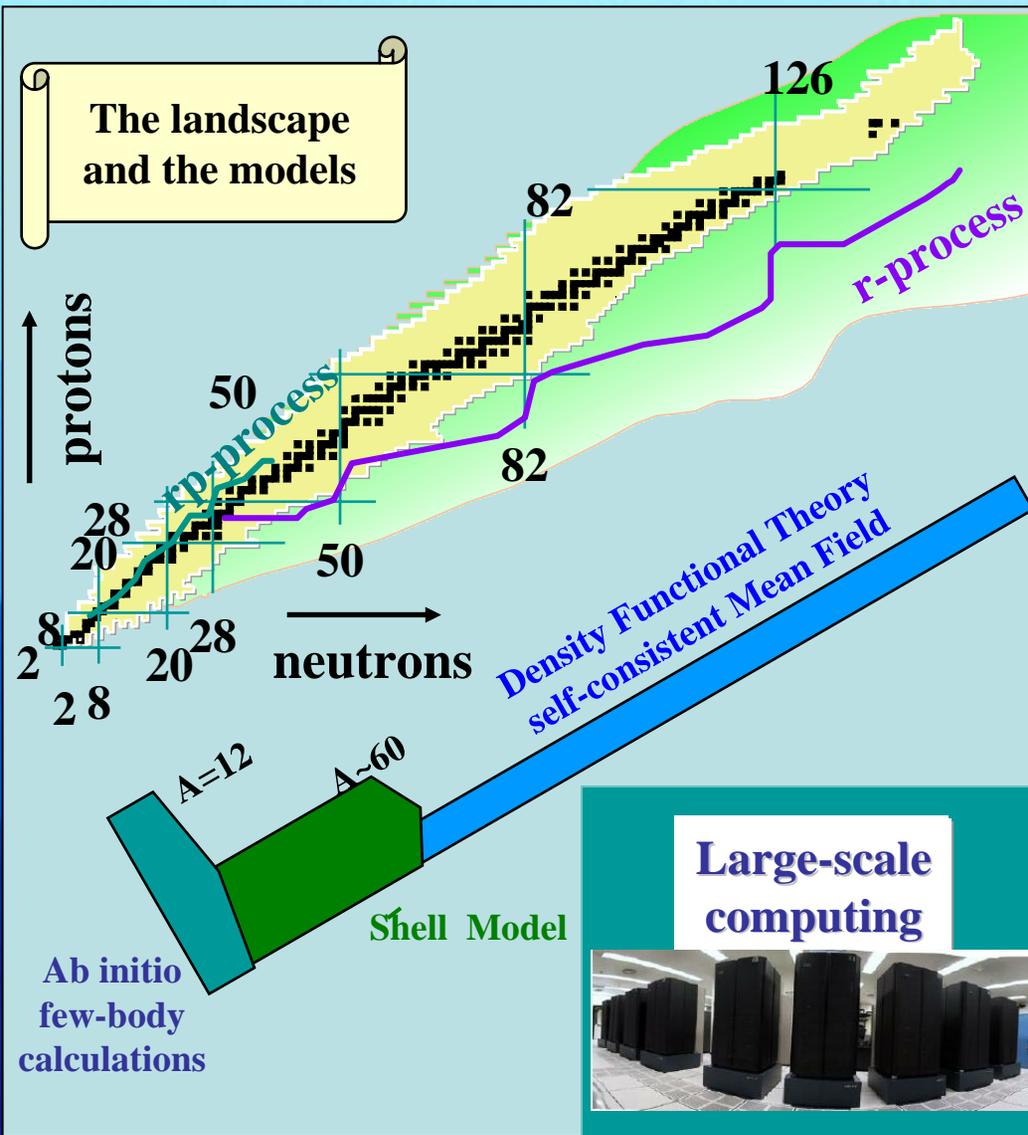
- **Microscopic nuclear structure**
- **Nucleon-nucleon effective field theory**
- **Microscopic energy density functional**
- **Coupling of nuclear structure and reaction theory**
- **Nuclear dynamics and symmetries of complex nuclei**

Nuclear astrophysics developments

- **Quantitative understanding of supernova**
- **Nuclear physics of gamma-ray bursts**
- **Neutrino astrophysics**
- **Neutron-star structure**

The nuclear quantum many-body problem underlies all of the structure/reaction developments and impacts our understanding of astrophysics, SBSS, and other applications.

Theoretical developments for the big questions



Main theory goals:

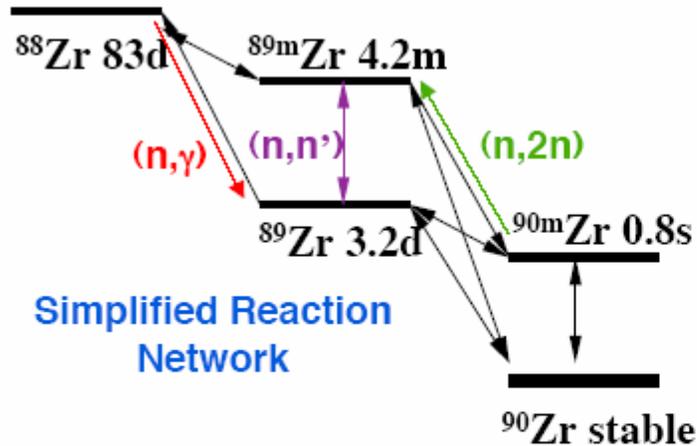
- Identify/investigate many-body methods that will extend to RIA
- Generate effective interactions
- **Make reliable predictions**
- Guide experimental efforts
- Use NN and 3N forces to build nuclei

Various approaches to low-energy nuclear theory:

- Coupled-cluster theory
- Shell Model Monte Carlo
- DMRG/Factorization
- Shell model diagonalization
- Continuum shell models
- HFB
- QRPA
- TDHF

Examples the importance of nuclear theory in other areas

From a talk by Ed Hartouni (LLNL):



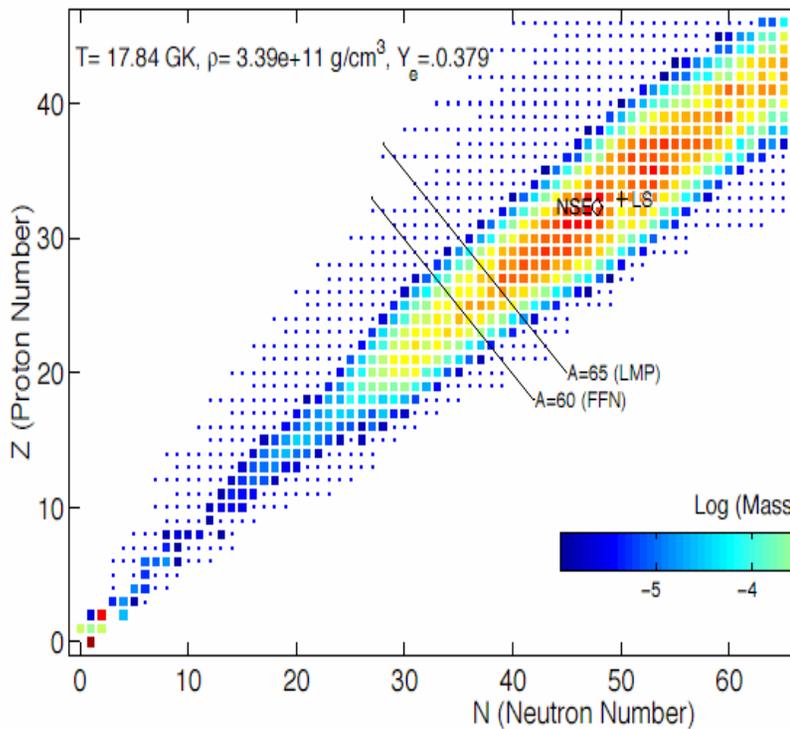
Example – Load ^{90}Zr

1. Neutron flux causes nuclear reactions (nucleosynthesis).
2. Measure ratios such as $^{88}\text{Zr}/^{89}\text{Zr}$ (radiochemistry).
3. Compare with calculated value from simulation (stewardship).

- Almost all isotopes in networks are unstable.
- Most reactions have no experimental data. (Zirconium network – 60 reactions, 5 examined experimentally).

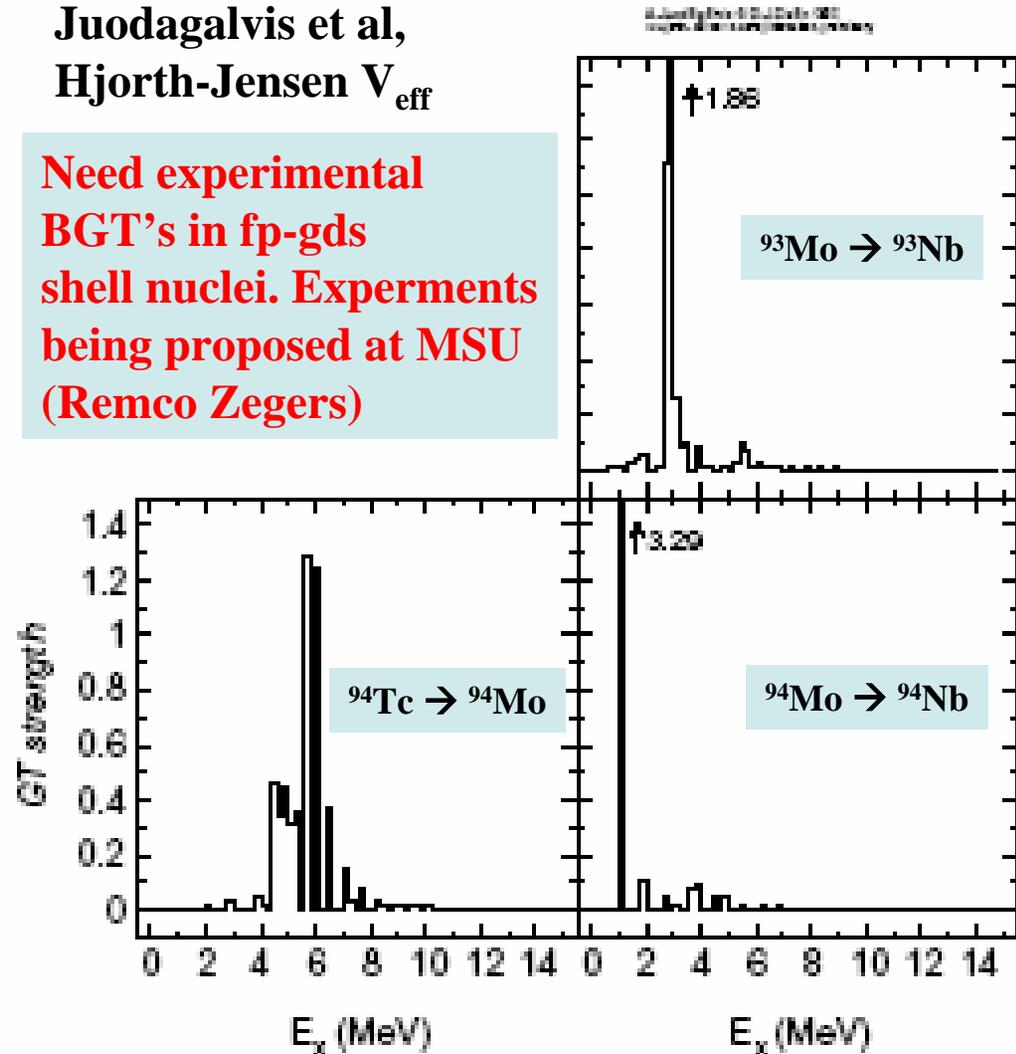
Astrophysical applications: core collapse supernovae

Mass trajectory during collapse



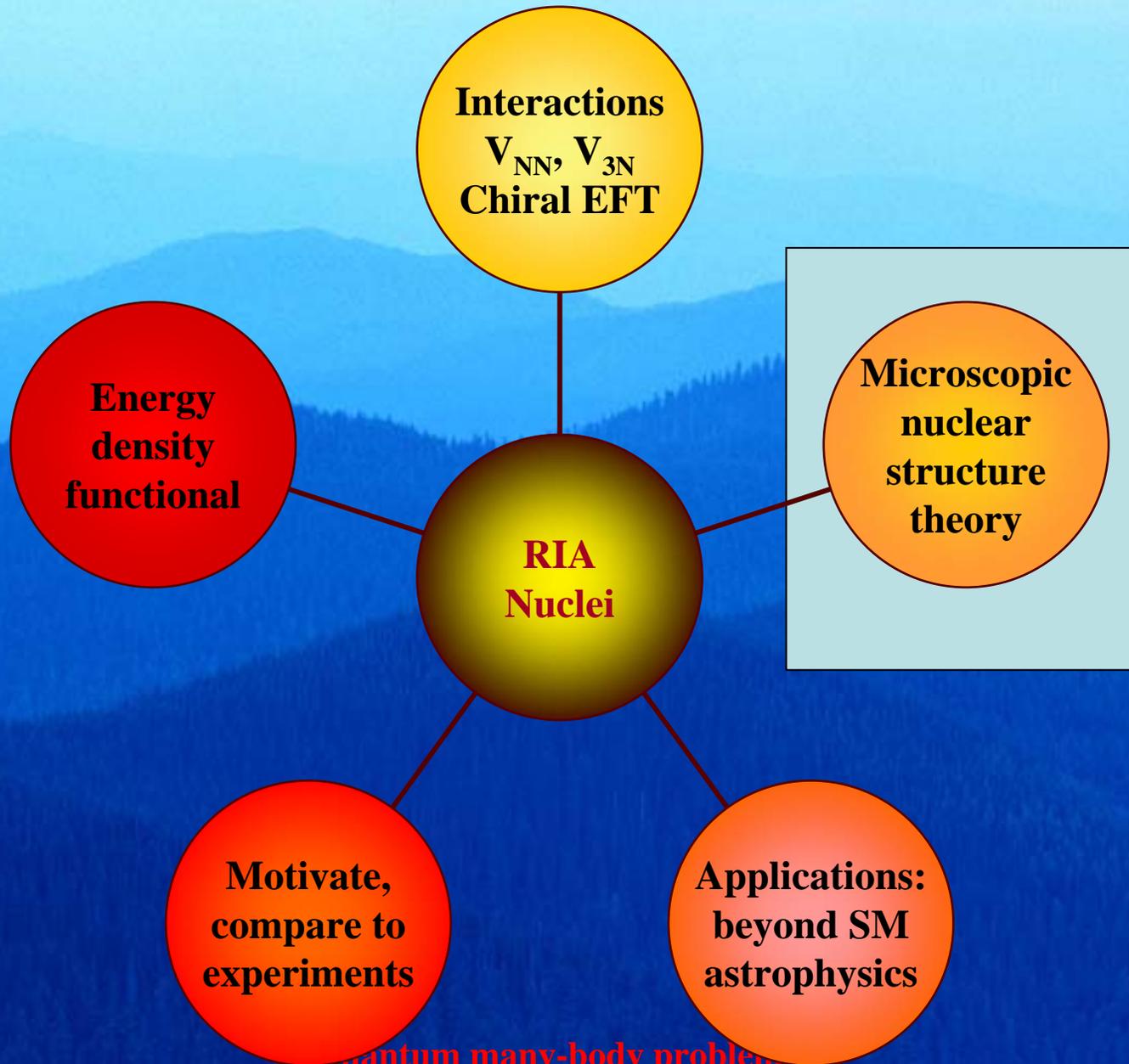
Juodagalvis et al,
Hjorth-Jensen V_{eff}

Need experimental
BGT's in fp-gds
shell nuclei. Experiments
being proposed at MSU
(Remco Zegers)



See: Langanke, Kolbe, Dean, PRC63, 032801R (2001)
Langanke et al (PRL, 2003) (rates calculation)
Hix et al (PRL, 2003) (core collapse implications)

Broad approach



Steps toward solutions

Begin with a bare NN (+3N) Hamiltonian

$$H = -\frac{\hbar}{2} \sum_{i=1}^A \frac{\nabla_i^2}{m_i} + \frac{1}{2} \sum_{i<j} V_{2N}(\vec{r}_i, \vec{r}_j) + \frac{1}{6} \sum_{i<j<k} V_{3N}(\vec{r}_i, \vec{r}_j, \vec{r}_k)$$

Bare (GFMC)

Basis expansion

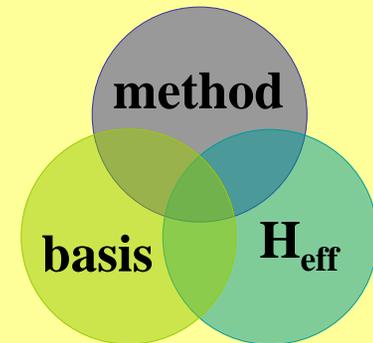
Basis expansions:

- Choose the method of solution
- Determine the appropriate basis
- Generate H_{eff}

Nucleus	4 shells	7 shells
4He	4E4	9E6
8B	4E8	5E13
12C	6E11	4E19
16O	3E14	9E24

Oscillator
single-particle
basis states

Many-body
basis states



Many-body problems

The ORNL-Oslo-MSU collaboration on nuclear many-body problems

OAK RIDGE NATIONAL LABORATORY

David Dean (CC methods for nuclei and extensions to V_{3N})
Thomas Papenbrock
David Bernholdt (Computer Science and Mathematics)
Trey White, Kenneth Roche (Computational Science)

MICHIGAN STATE
UNIVERSITY

Department of
Chemistry

Piotr Piecuch (CC methods in chemistry and extensions)
Karol Kowalski (to PNNL)
Marta Wloch
Jeff Gour



UNIVERSITY
OF OSLO

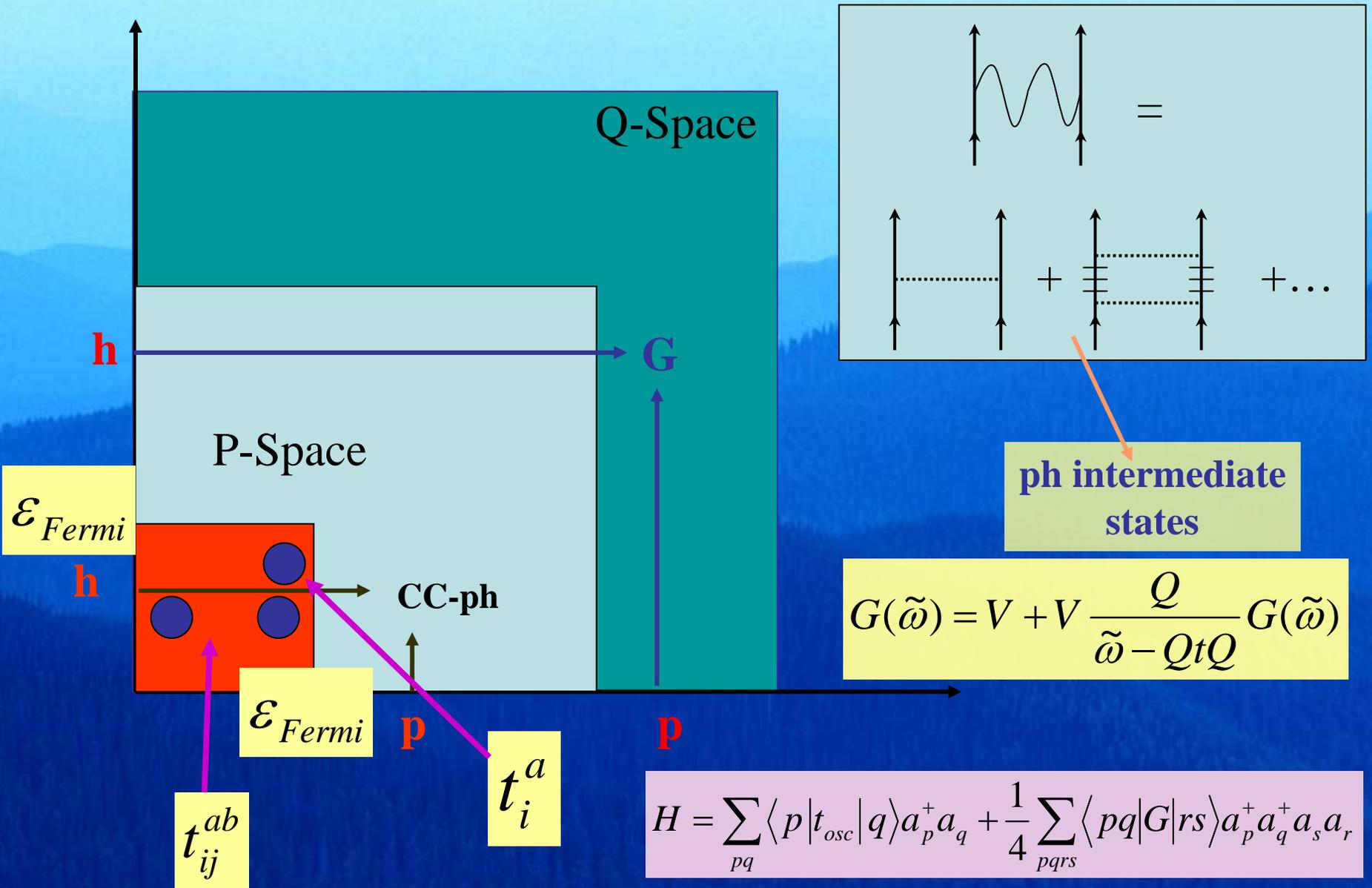
Morten Hjorth-Jensen (Effective interactions)
Maxim Kartamychev (3-body forces in nuclei)
Gaute Hagen (effective interactions for weakly bound systems)

Research Plan

- Excited states (!)
- Observables (!)
- Triples corrections (!)
- Open shells
- V_{3N}
- $50 < A < 100$
- Reactions
- TD-CCSD??

Quantum many-body problems

Choice of model space and the G-matrix



Diagonalization: configuration-interaction, interacting shell model

Yields eigenfunctions which are linear combinations of particle-hole amplitudes

$$|\Psi_\alpha\rangle = \left(1 + b_i^a a_a^+ a_i + b_{ij}^{ab} a_a^+ a_b^+ a_i a_j + \dots\right) |\Phi_0\rangle$$

1p-1h

2p-2h

Advantages (NCSM,...)

- Detailed spectroscopic information available
- Wave functions calculated and stored

Disadvantages

- Dimension of problem increases dramatically with the number of active particles (combinatorial growth).
- Disconnected diagrams enter if truncated

Fascinating many-body approach that promises to push us to medium mass nuclei: Coupled Cluster Theory

Some interesting features of CCM:

- **Fully microscopic**
- **Size extensive:**
only linked diagrams enter
- **Size consistent:**
relevant for reactions
- **Capable of systematic improvement**
- **Amenable to parallel computing**

N=8 run, total compute time = 1.9 Tf-hours (ORNL and NERSC)

Scaling to ^{40}Ca , $N = 9: O(n_u^4 n_o^2): 72 \text{ Tf - hours}$

A short history

Formal introduction:

1958: Coester, Nucl. Phys. 7, 421

1960: Coester and Kummel, Nucl. Phys. 17, 477

Introduction into Chemistry (late 60's):

1971: Cizek and Paldus, Int. J. Quantum Chem. 5, 359

Numerical implementations

1978: Pople et al., Int. J. Quantum Chem Symp, 14, 545

1978: Bartlett and Purvis, Int. J. Quantum Chem 14, 561

Initial nuclear calculations (1970's):

1978: Kummel, Luhrmann, Zabolitzky, Phys. Rep. 36, 1 and refs. therein

1980-90s: Bishop's group. Coordinate space.

Few applications in nuclei, explodes in chemistry and molecular sciences.

Hard-core interactions; computer power; unclear interactions

Nuclear physics reintroduction: ($1/E_{ph}$ expansion)

1999: Heisenberg and Mihiala, Phys. Rev. C59, 1440; PRL84, 1403 (2000)

Three nuclei; JJ coupled scheme; bare interactions, approximate V_{3N}

Useful References

Crawford and Schaefer, Reviews in Computational Chemistry, 14, 336 (2000)

Bartlett, Ann. Rev. Phys. Chem. 32, 359 (1981)

Coupled Cluster Theory

$$|\Psi\rangle = \exp(T)|\Phi\rangle$$

**Correlated Ground-State
wave function**

**Correlation
operator**

**Reference Slater
determinant**

$$T = T_1 + T_2 + T_3 + \dots$$

$$T_1 = \sum_{\substack{i < \varepsilon_f \\ a > \varepsilon_f}} t_{ai} a_a^+ a_i$$

$$T_2 = \sum_{\substack{ij < \varepsilon_f \\ ab > \varepsilon_f}} t_{abij} a_a^+ a_b^+ a_j a_i$$

Energy

$$E = \langle \Phi | \exp(-T) H \exp(T) | \Phi \rangle$$

Amplitude equations

$$\langle \Phi_{ij\dots}^{ab\dots} | \exp(-T) H \exp(T) | \Phi \rangle = 0$$

• Nomenclature

- Coupled-clusters in singles and doubles (CCSD)
- ...with triples corrections CCSD(T);

Dean & Hjorth-Jensen, PRC69, 054320 (2004); Kowalski, Dean, Hjorth-Jensen, Papenbrock, Piecuch, PRL92, 132501 (2004)

Derivation of CC equations

Use Baker-Hausdorff

$$\exp(-T)H \exp(T) = H + [H, T_1] + [H, T_2] + \frac{1}{2} [[H, T_1], T_1] + \frac{1}{2} [[H, T_2], T_2] + [[H, T_1], T_2] + \dots$$

Terminates at quadruply nested commutators (for $H=H_1+H_2$) for all T.

Normal order the Hamiltonian

$$H = \sum_{pq} f_{pq} \{a_p^+ a_q\} + \frac{1}{4} \sum_{pqrs} \langle pq || rs \rangle \{a_p^+ a_q^+ a_s a_r\} + \sum_i \langle i | t_{osc} | i \rangle + \frac{1}{2} \sum_{ij} \langle ij || ij \rangle$$

$$f_{pq} = \langle p | t_{osc} | q \rangle + \sum_i \langle pi || qi \rangle$$

Fock operator


$$\langle \Phi_0 | H | \Phi_0 \rangle$$

Derivation of CC equations

T₁ amplitudes from: $\langle \Phi_i^a | \exp(-T) H \exp(T) | \Phi \rangle = 0$

$$\begin{aligned}
 0 = & f_{ai} + \sum_c f_{act_i^c} - \sum_k f_{kit_k^a} + \sum_{kc} \langle ka || ci \rangle t_k^c + \sum_{kc} f_{ket_{ik}^{ac}} + \frac{1}{2} \sum_{ked} \langle ka || cd \rangle t_{ki}^{cd} - \\
 & \frac{1}{2} \sum_{klc} \langle kl || ci \rangle t_{kl}^{ca} - \sum_{kc} f_{ket_i^c t_k^a} - \sum_{klc} \langle kl || ci \rangle t_k^c t_l^a + \sum_{ked} \langle ka || cd \rangle t_k^c t_i^d - \quad [152] \\
 & \sum_{klcd} \langle kl || cd \rangle t_k^c t_i^d t_l^a + \sum_{klcd} \langle kl || cd \rangle t_k^c t_{li}^{da} - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{ki}^{cd} t_l^a - \frac{1}{2} \sum_{klcd} \langle kl || cd \rangle t_{kl}^{ca} t_i^d,
 \end{aligned}$$

Note T₂ amplitudes also come into the equation.

T₂ amplitudes from:

$$\langle \Phi_{ij}^{ab} | \exp(-T) H \exp(T) | \Phi \rangle = 0$$

$$0 = \langle ab || ij \rangle + \sum_c (f_{bc} t_{ij}^{ac} - f_{ac} t_{ij}^{bc}) - \sum_k (f_{kj} t_{ik}^{ab} - f_{ki} t_{jk}^{ab}) + \quad [153]$$

$$\frac{1}{2} \sum_{kl} \langle kl || ij \rangle t_{kl}^{ab} + \frac{1}{2} \sum_{cd} \langle ab || cd \rangle t_{ij}^{cd} + P(ij) P(ab) \sum_{kc} \langle kb || cj \rangle t_{ik}^{ac} +$$

$$P(ij) \sum_c \langle ab || cj \rangle t_i^c - P(ab) \sum_k \langle kb || ij \rangle t_k^a +$$

$$\frac{1}{2} P(ij) P(ab) \sum_{kled} \langle kl || cd \rangle t_{ik}^{ac} t_{lj}^{db} + \frac{1}{4} \sum_{kled} \langle kl || cd \rangle t_{ij}^{cd} t_{kl}^{ab} -$$

$$P(ab) \frac{1}{2} \sum_{kled} \langle kl || cd \rangle t_{ij}^{ac} t_{kl}^{bd} - P(ij) \frac{1}{2} \sum_{kled} \langle kl || cd \rangle t_{ik}^{ab} t_{jl}^{cd} +$$

$$P(ab) \frac{1}{2} \sum_{kl} \langle kl || ij \rangle t_k^a t_l^b + P(ij) \frac{1}{2} \sum_{cd} \langle ab || cd \rangle t_i^c t_j^d - P(ij) P(ab) \sum_{kc} \langle kb || ic \rangle t_k^a t_j^c +$$

$$P(ab) \sum_{kc} f_{kc} t_k^a t_{ij}^{bc} + P(ij) \sum_{kc} f_{kc} t_i^c t_{jk}^{ab} -$$

$$P(ij) \sum_{kle} \langle kl || ci \rangle t_k^c t_{lj}^{ab} + P(ab) \sum_{kcd} \langle ka || cd \rangle t_k^c t_{ij}^{db} +$$

$$P(ij) P(ab) \sum_{kod} \langle ak || dc \rangle t_i^d t_{jk}^{bc} + P(ij) P(ab) \sum_{kle} \langle kl || ic \rangle t_i^a t_{jk}^{bc} +$$

$$P(ij) \frac{1}{2} \sum_{kle} \langle kl || cj \rangle t_i^c t_{kl}^{ab} - P(ab) \frac{1}{2} \sum_{kod} \langle kb || cd \rangle t_k^a t_{ij}^{cd} - P(ij) P(ab) \frac{1}{2} \sum_{kcd} \langle kb || cd \rangle t_i^c t_k^a t_j^d + P(ij) P(ab) \frac{1}{2} \sum_{kle} \langle kl || cj \rangle t_i^c t_k^a t_l^b -$$

$$P(ij) \sum_{kled} \langle kl || cd \rangle t_k^c t_i^d t_{lj}^{ab} - P(ab) \sum_{kled} \langle kl || cd \rangle t_k^c t_l^a t_{ij}^{db} +$$

$$P(ij) \frac{1}{4} \sum_{kled} \langle kl || cd \rangle t_i^c t_j^d t_{kl}^{ab} + P(ab) \frac{1}{4} \sum_{kled} \langle kl || cd \rangle t_k^a t_l^b t_{ij}^{cd} +$$

$$P(ij) P(ab) \sum_{kled} \langle kl || cd \rangle t_i^c t_l^b t_{kj}^{ad} + P(ij) P(ab) \frac{1}{4} \sum_{kled} \langle kl || cd \rangle t_i^c t_k^a t_j^d t_l^b.$$

**Nonlinear terms in t₂
(4th order)**

$$P(ij) f(ij) = f(ij) - f(ji)$$

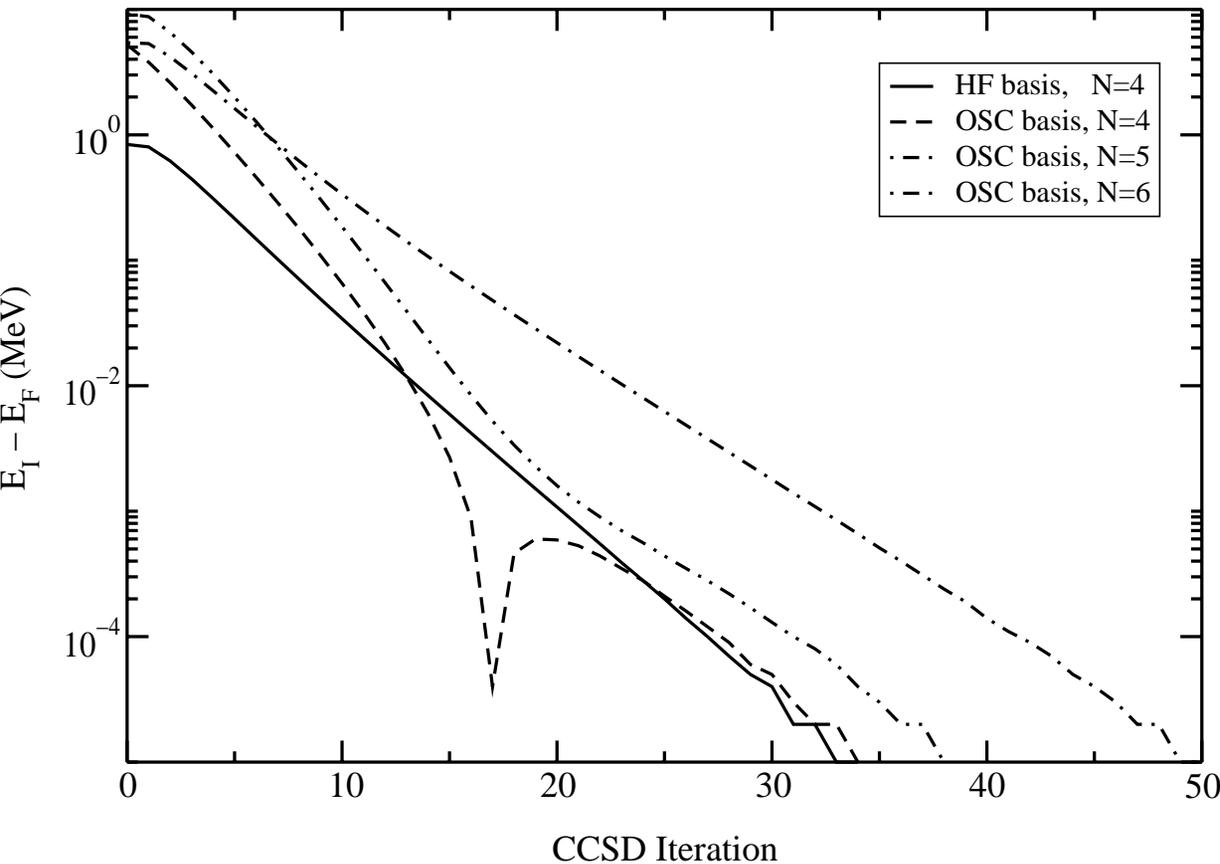
**An interesting mess.
But solvable....**

Iterative solution

On the first iteration: use first and second-order many-body perturbation theory as a guide. This gives:

$$= f_{ai} / D_i^a$$

$$= \langle ab || ij \rangle / D_{ij}^{ab}$$

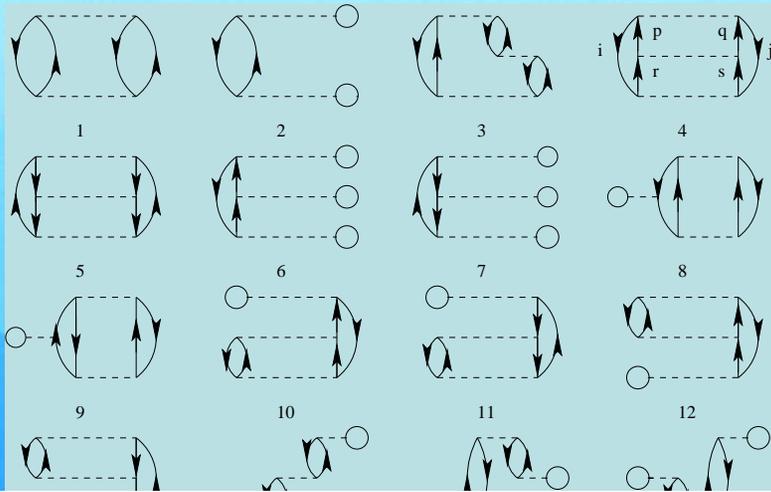


Insert into the RHS and
compute new amplitudes

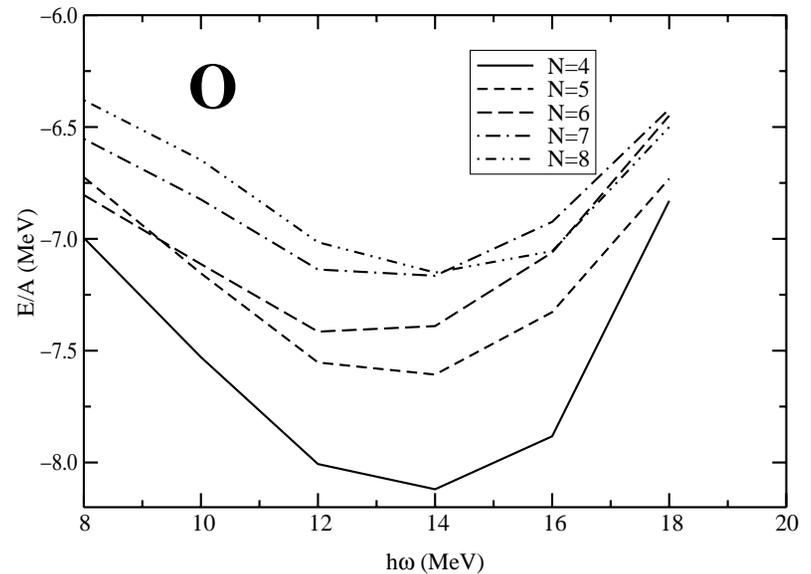
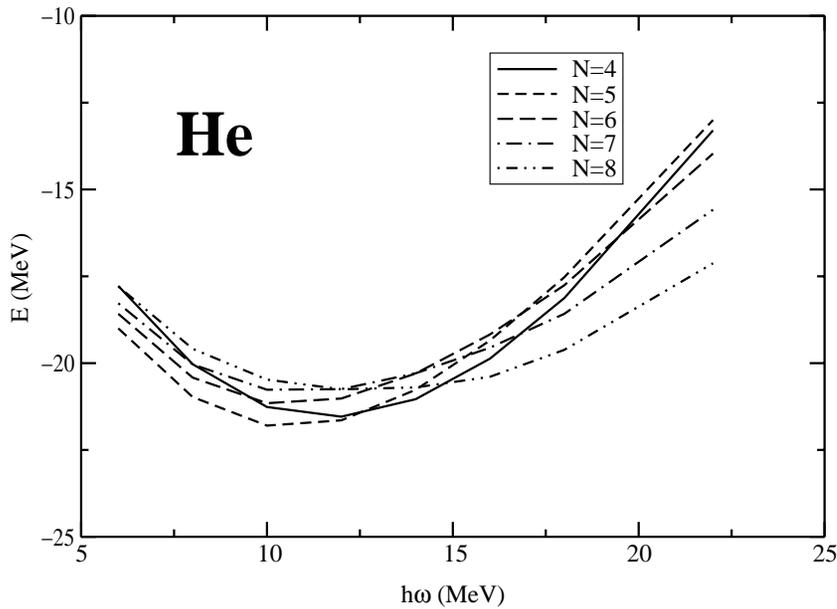
Continue until
convergence

Compare: HF vs OSC:
39.31 MeV (OSC)
38.47 MeV (HF)
2.1% difference

CCSD and MBPT results to third order



N (hw)	E(0)	E^{2nd} (MBPT)	E^{3rd} (MBPT)	E(F)
4 (14)	-135.12	-132.06	-129.92	-140.47
5 (14)	-124.79	-124.84	-121.52	-127.79
6 (14)	-121.36	-121.48	-118.23	-119.73



Comparison of HF and OSC basis (Idaho-A)

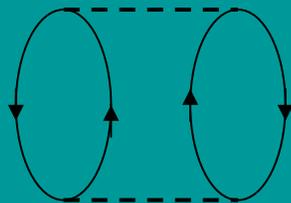
	E_{corr}	Term 1	Term 2	Term 3	E_0	$\langle H \rangle$
OSC	-29.865	-9.669	-1.757	-18.439	-109.45	-139.31
HF	-16.498	7.0e-6	-0.3e-3	-16.498	-121.98	-138.47

$$E_{\text{corr}} = E_{\text{ccsd}} - E_0 = \sum_{ia} f_{ia} t_i^a + \frac{1}{2} \sum_{aibj} \langle ij || ab \rangle t_i^a t_j^b + \frac{1}{4} \sum_{aibj} \langle ij || ab \rangle t_{ij}^{ab}$$

Changing the basis hardly affects the solutions.

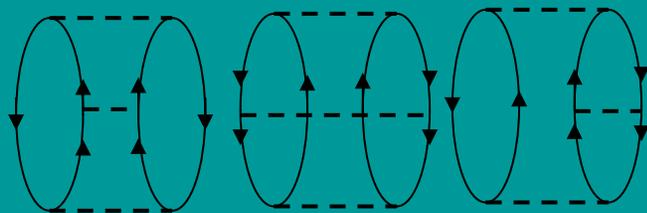
Correspondence with MBPT

2nd order



$$t_{ij}^{ab}(1) = \langle ab || ij \rangle / D_{ijab}$$

$$E_2 = \sum_{\substack{a>b \\ i>j}} \langle ab || ij \rangle t_{ij}^{ab}(1)$$



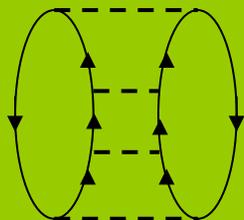
3rd order

$$t_{ij}^{ab}(2) = \frac{1}{2} \sum_{kl} \langle kl || ij \rangle t_{kl}^{ab}(1) +$$

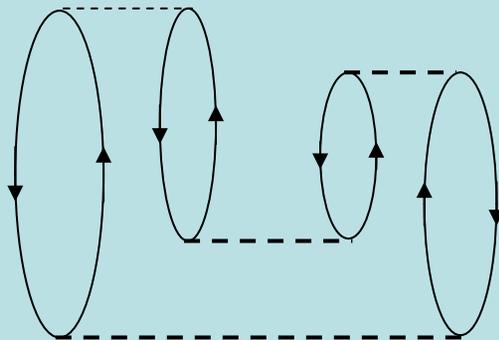
$$\frac{1}{2} \sum_{cd} \langle ab || cd \rangle t_{ij}^{cd}(1) + P(ij)P(ab) \sum_{kc} \langle kb || cj \rangle t_{ik}^{ac}(1)$$

$$E_3 = \sum_{\substack{a>b \\ i>j}} \langle ab || ij \rangle t_{ij}^{ab}(2)$$

A few more diagrams



+ all diagrams of this kind (11 more) 4th order
[replace $t(2)$ and repeat above 3rd order calculation]



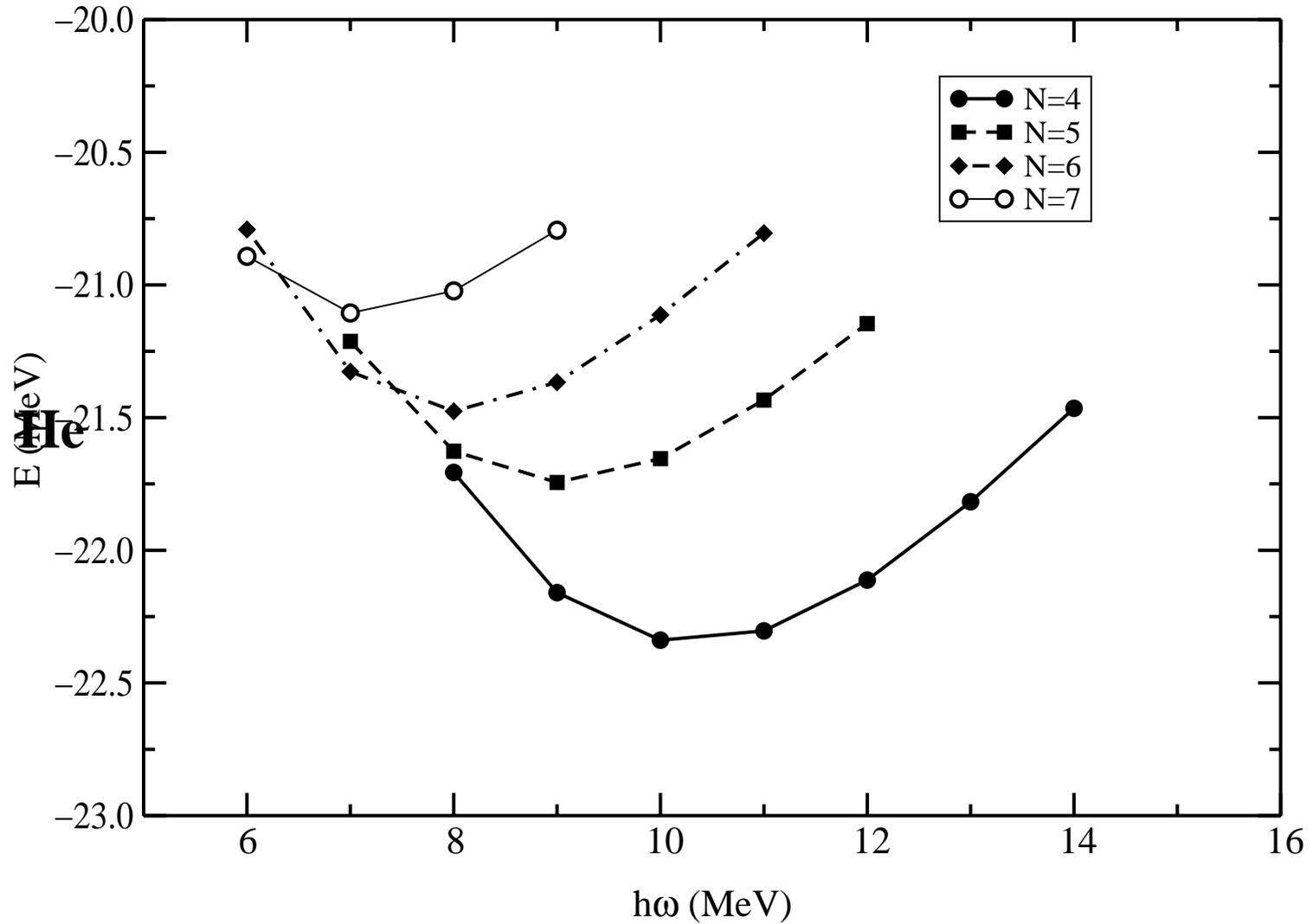
+ all diagrams of this kind (6 more) 4th order

$$t_{ij}^{ab}(3; N) = \frac{1}{2} P(ij) P(ab) \sum_{klcd} \langle kl || cd \rangle t_{ik}^{ac}(1) t_{lj}^{db}(1) + \frac{1}{4} \sum_{klcd} \langle kl || cd \rangle t_{ij}^{cd}(1) t_{kl}^{ab}(1)$$

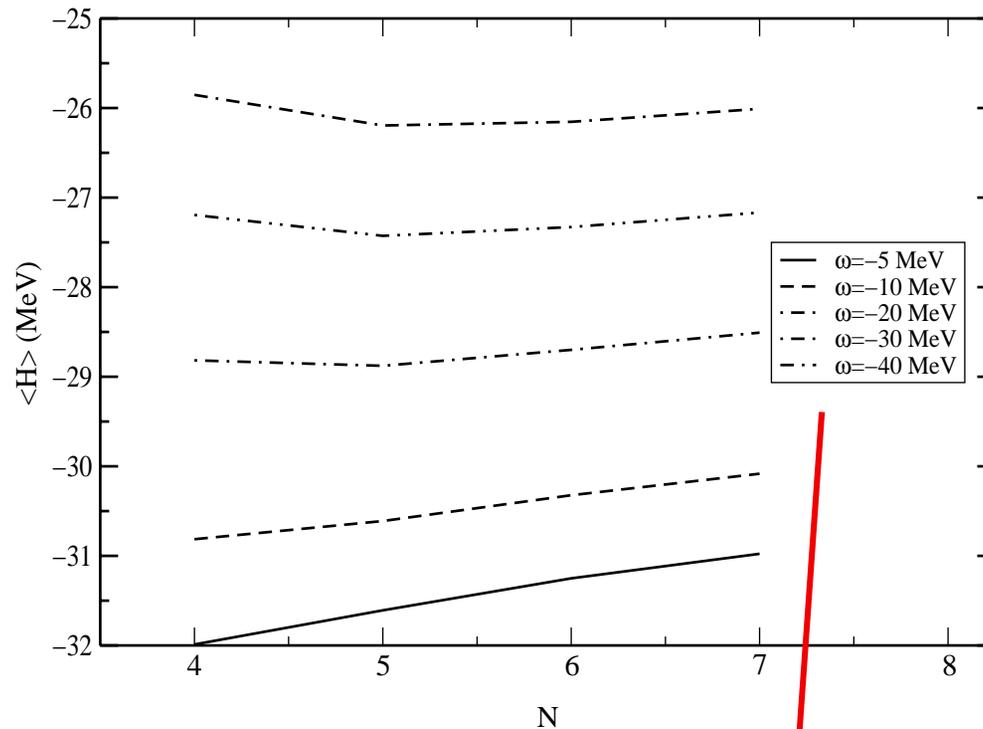
$$- \frac{1}{2} P(ab) \sum_{klcd} \langle kl || cd \rangle t_{ij}^{ac}(1) t_{kl}^{bd}(1) - \frac{1}{2} P(ij) \sum_{klcd} \langle kl || cd \rangle t_{ik}^{ab}(1) t_{jl}^{cd}(1)$$

$$E_4^Q = \sum_{\substack{a>b \\ i>j}} \langle ab || ij \rangle t_{ij}^{ab}(3; N)$$

Ground states of helium and oxygen



Ground state of helium: Idaho-A



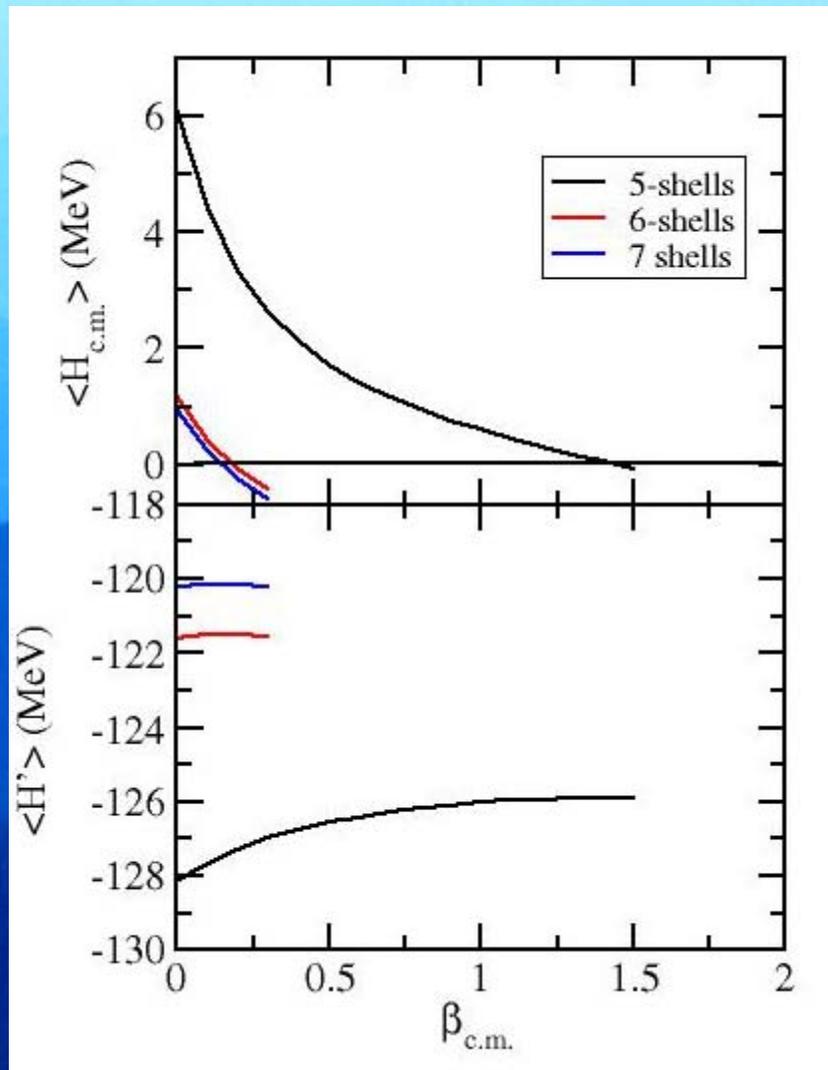
We also investigated:

$$H \leftarrow H + \beta_{c.m.} H_{c.m.}$$

$$H \leftarrow H - T_{c.m.} + \beta_{c.m.} H_{c.m.}$$

Need for similarity transformed H_{eff} (undearway).

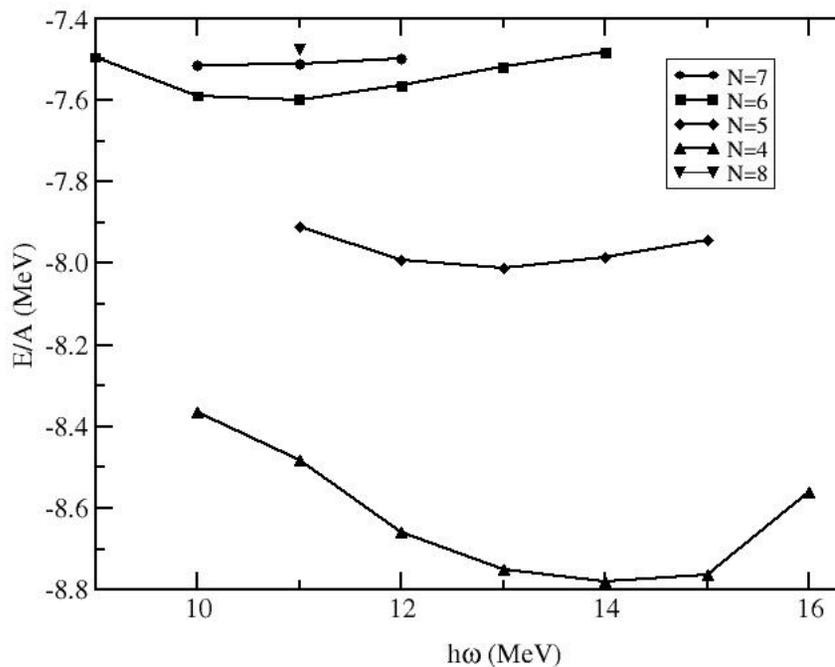
Another center of mass correction on ^{16}O



$$H' = H + \beta_{c.m.} H_{c.m.}$$

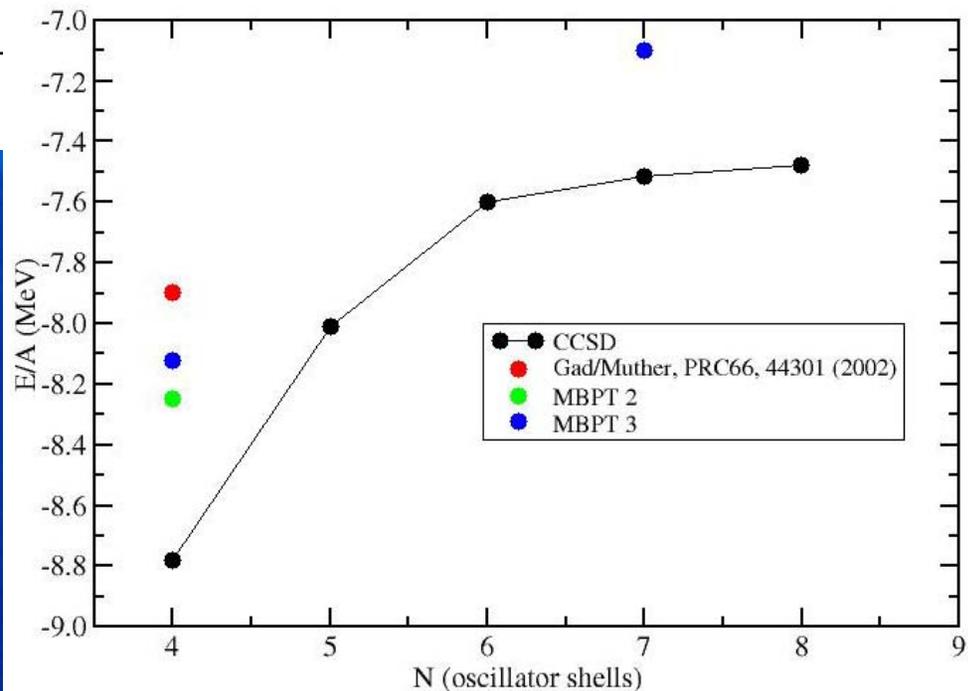
**Controls COM
contamination of both
ground and excited states.
Used to isolate “REAL” states.**

Calculations for ^{16}O



Reasonably converged

- Idaho-A: No Coulomb
- Coulomb: +0.7 MeV
- Expt result is -8.0 MeV/A

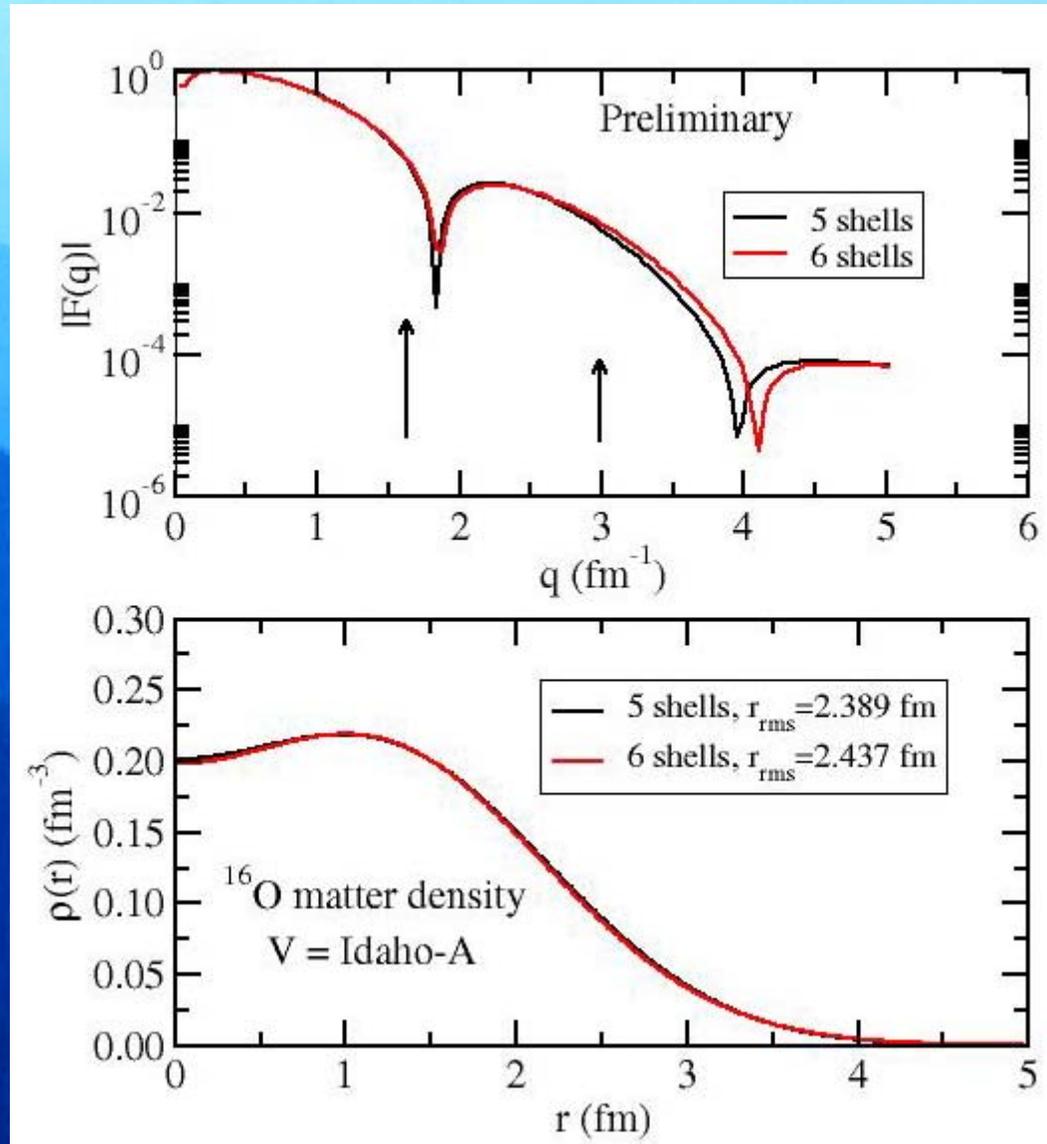


Nuclear Properties

$$H = H + \lambda\Omega$$

$$\langle \Omega \rangle = \frac{dE}{d\lambda}$$

Can also be done as
a solution to the CCSD
left eigenvalue problem
yields density matrix.

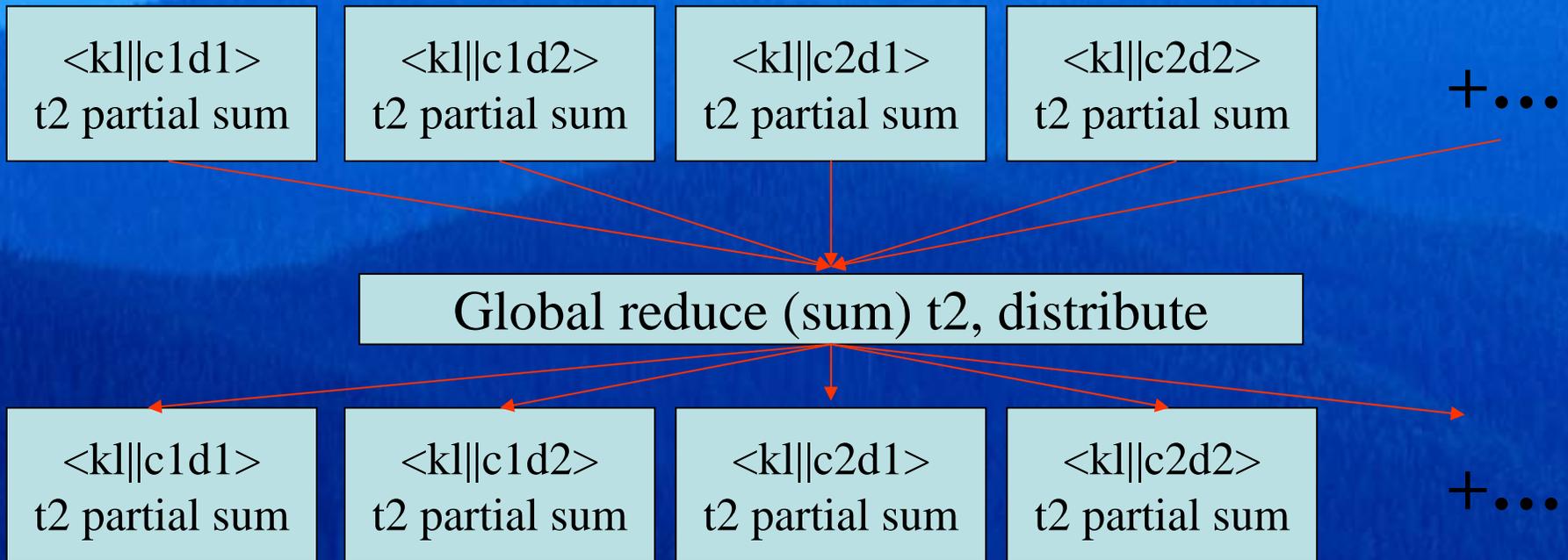


Some aspects of our (Dean/Hjorth-Jensen) CCSD code

Memory distributed across processors

$$f(ab, ij) = \sum_{\substack{kl < \varepsilon_f \\ cd > \varepsilon_f}} \langle kl || cd \rangle t_{ij}^{cd} t_{kl}^{ab}$$

Partial sum t_2 resides on each processor



Some coding aspects

$$f(ab, ij) = \sum_{\substack{kl < \varepsilon_f \\ cd > \varepsilon_f}} \langle kl \| cd \rangle t_{ij}^{cd} t_{kl}^{ab}$$

$$\alpha = (a, b), \beta = (k, l), \gamma = (c, d), \delta = (i, j)$$

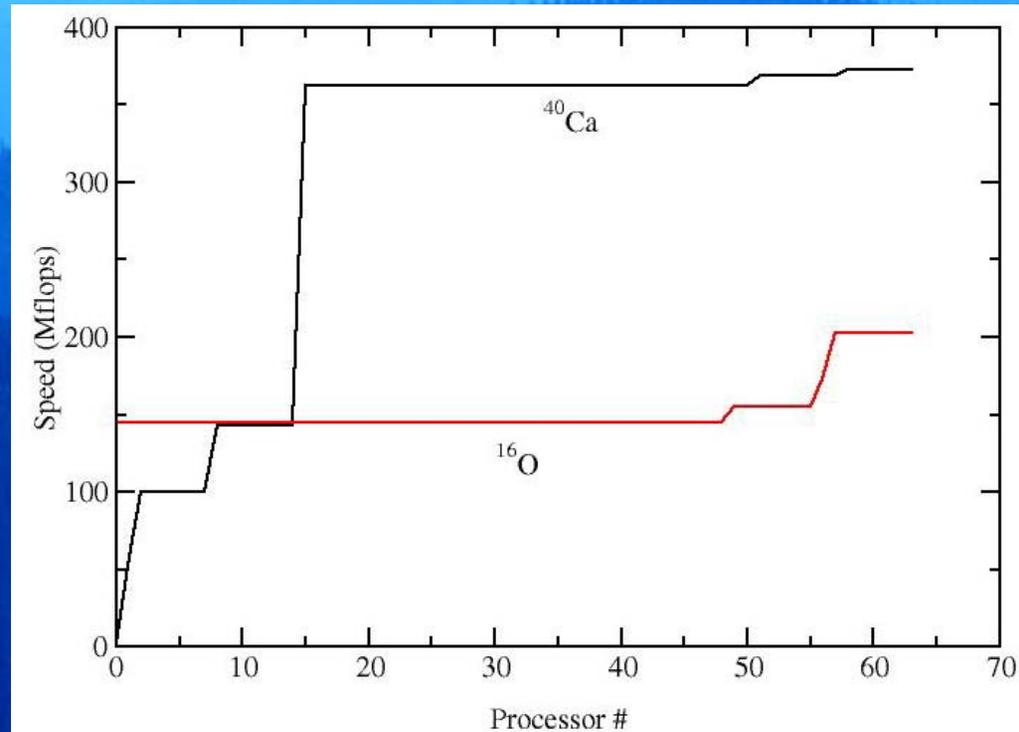
$$M_{\alpha, \beta} = t_{kl}^{ab}$$

$$N_{\beta, \gamma} = \langle kl \| cd \rangle$$

$$O_{\gamma, \delta} = t_{ij}^{cd}$$

$$Q_{\alpha, \delta} = f(ab, ij)$$

$$P = M \cdot N \quad Q = P \cdot O \quad f \leftarrow Q$$

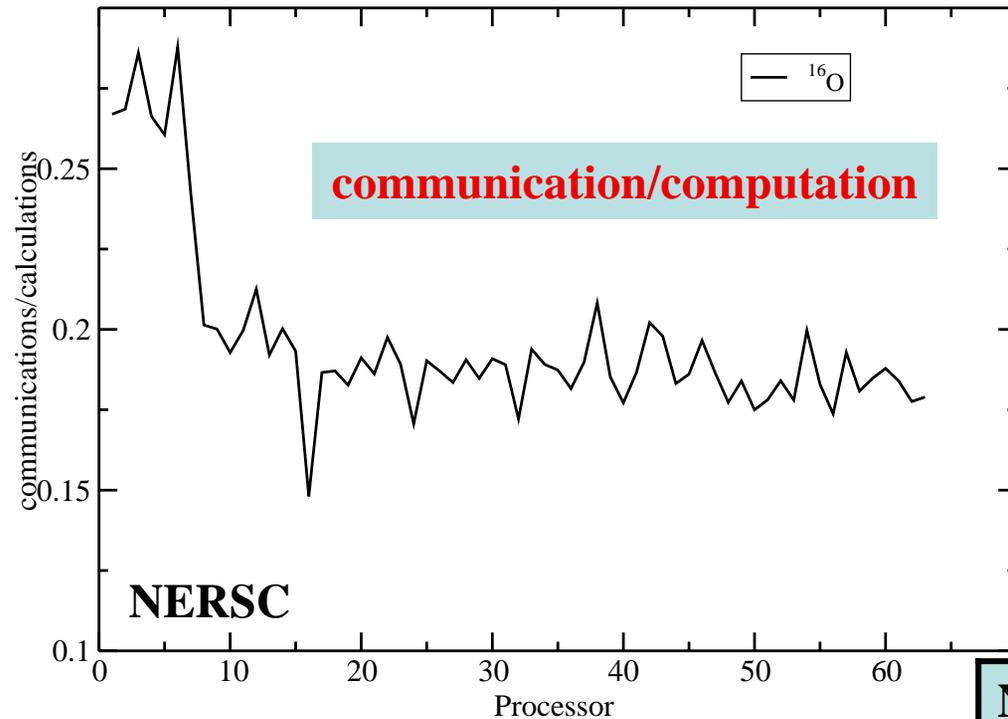


Very fast:

BLAS implementation

Calculations performed at NERSC

Some more properties of the parallel implementation



NERSC=1.5 Gflop (peak)/processor
 ORNL=5.8 Gflop (peak)/processor

N=8 run performed on ORNL
 Altix system (RAM) using 100
 processors at 1.8 Gflop/processor
 (0.18 Tflop) sustained. Total compute
 time = 1.9 Tf-hours.

Scaling to ^{40}Ca : $O(n_u^4 n_o^2)$: 11.9 Tf - hours

N	N_s	^4He	G (x10 ⁶)	^{16}O
4	80	1792	0.165	24,960
5	140	4000	1.5	77,880
6	224	7,976	10.1	176,240
7	336	14,112	51	345k
8	480	---	212	604k

Correcting the CCSD results by non-iterative methods

Goal: Find a method that will yield the complete diagonalization result in a given model space

How do we obtain the triples correction?

How do our results compare with ‘exact’ results in a given model space, for a given Hamiltonian?

“Completely Renormalized Coupled Cluster Theory”

P. Piecuch, K. Kowalski, P.-D. Fan, I.S.O. Pimienta, and M.J. McGuire, Int. Rev. Phys. Chem. 21, 527 (2002)

Completely renormalized CC in one slide

CC generating functional

$$\Lambda_{CC}[\Psi] = \frac{\sum_{n=1}^N \langle \Psi | (H - E_0^{(A)}) e^{T(A)} | \Phi \rangle}{\langle \Psi | e^{T(A)} | \Phi \rangle}$$

T(A) = model correlation

if $\Psi \rightarrow \Psi_0$

then $\Lambda_{CC} = \delta = E_0 - E_0^{(A)}$

$$\delta = \frac{1}{36} \sum_{ijk, abc} \langle \tilde{\Psi} | \Phi_{abc}^{ijk} \rangle M_{ijk}^{abc} / \Delta$$

$$\Delta = \langle \tilde{\Psi} | e^{T(CCSD)} | \Phi \rangle$$

$$M_{abc}^{ijk} = \langle \Phi_{ijk}^{abc} | \bar{H}^{CCSD} | \Phi \rangle$$

$$|\tilde{\Psi}\rangle = Pe^{(T^{(CCSD)} + \tilde{T}_3)}$$

Different choices of Ψ will yield slightly different triples corrections

Leading order terms in the triples equation

Triples correction to the ground state energy He-4 (4 major oscillator shells)

Method	Energy (MeV)
-----	-----
CCSD	-21.978
CR-CCSD[T],I	-22.665
CR-CCSD[T],I/D=1	-23.214
CR-CCSD[T],II	-22.841
CR-CCSD[T],II/D=1	-23.524
Shell Model 2p-2h	-20.175
Shell Model 3p-3h	-22.235
FULL shell model	-23.484

Different many-body approaches to the energy denominator

Able to reproduce the exact result to within 0.08 MeV.

$$H' = H + \beta_{c.m.} H_{c.m.}$$

Triples correction and excited states by equation of motion CCSD He-4 (4 major oscillator shells)

$$\bar{H} = \exp(-T)H \exp(T)$$

Diagonalize in the space of 0,1,2 ph excitations

State	EOMCCSD	CR-CCSD(T)	Shell model	$\langle \beta_{\text{c.m.}} H_{\text{c.m.}} \rangle$
J=1	11.7913	12.044	11.465	8.2
J=0	21.2033	21.489	21.569	0.8
J=2	22.435	22.650	22.697	14.3

**Follows similar formalism
for excited states as in previous slide.**

^{16}O in four major oscillator shells

Method	Energy (MeV)
CCSD	-139.310
CR-CCSD(T),a	-139.465
CR-CCSD(T),a/D=1	-139.621
CR-CCSD(T),b	-139.375
CR-CCSD(T),b/D=1	-139.440
CR-CCSD(T),c	-139.391
CR-CCSD(T),c/D=1	-139.467
Shell model 2p-2h	-131.887
Shell model 3p-3h	-135.489
Shell model 4p-4h	-138.387

1) Relative size of terms:

a) T_1 and T_2 of similar order

b) $T_1 T_2$ disconnected

>> T_3 connected triples

c) diff between 2p-2h shell model

and CCSD comes mainly from $T_1 T_2$

d) If T_3 were large CCSD(T)

would be far below CCSD

2) Size extensive nature of CC

3) CCSD + CR-CCSD(T) bring

$T_1^3 T_2$, $T_1 T_2^2$, T_2^3 not in the 4p-4h shell model

4) Scaling

$$\text{CCSD} : n_o^2 n_u^4$$

$$\text{CCSD(T)} : n_o^3 n_u^4$$

$$4p - 4h \text{ shell model} : n_o^4 n_u^6$$

Conclusions and Perspectives

- Solution of the nuclear many-body problems requires extensive use of computational and mathematical tools. Numerical analysis becomes extremely important; methods from other fields (chemistry, CS) invaluable.
- Detailed investigation of triples corrections via CR-CCSD(T) indicates convergence at the triples level (in the small space) for both He and O calculations. Promising result.
- Excited states calculated for the first time using EOMCCSD in ${}^4\text{He}$ (${}^{16}\text{O}$ coming)
- ${}^{16}\text{O}$ nearly converged at 8 oscillator shells (shells, not Nhw).
- Continuing work on the interaction; efforts to move to similarity transformed G are underway.
- Open shell systems is the next big algorithmic step; EOMCCSD for larger model spaces underway; Ca-40 underway; V_{3N} beginning

RIA Theory Group

Rare Isotope Accelerator Project (RIA)

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[RIATG MEETING 31 OCTOBER, Chicago.](#)

The RIATG is a group of over 140 scientists that was formed following the 2002 Fall DNP meeting held in East Lansing. The primary purpose of RIATWG is to organize the nuclear theory community interested in RIA physics to:

- Identify and prioritize the most important physics questions to be addressed at RIA
- Act as a forum and a voice for the nuclear structure and astrophysics theory community to most effectively enhance the nuclear theory effort in the US. This follows from the charge in the long-range plan to "Significantly increase funding for nuclear theory, which is essential for the developing potential of the scientific program".
- Partner with the RIA Users Group and the RIA steering committee to promote RIA

Breaking News

Posted June 4, 2004: Election for Executive Committee Results [...more](#)

April 6, 2004: Nominations Committee formed, charter created. [...more](#)

March 12: RIA Theory Group approves charter [...more](#)

[Final report](#) of the NSAC Subcommittee on Nuclear Theory

[Presentations](#) from the Workshop of the RIA Theory Working Group available